International Journal of
Quantum Chemistry

Contents for Volume 61, 1997

Issue No. 1, 1997

Editorial v

Theoretical and Computational Developments

Symmetric Group Approach to Relativistic CI. I. General Formalism
N. Flocke, M. Barysz, J. Karwowski, and G. H. F. Diercksen 1

Symmetric Group Approach to Relativistic CI. II. Reduction of Matrices in the Spin Space
N. Flocke, M. Barysz, J. Karwowski, and G. H. F. Diercksen 11

Symmetric Group Approach to Relativistic CI. III. Matrix Elements for Spin-Dependent Operators
N. Flocke, M. Barysz, J. Karwowski, and G. H. F. Diercksen 21

Using Full-CI Algorithms in Bethe–Goldstone-Type Expansions of the Correlation Energy
A. Povill and J. Rubio 35

Unexpected CASSCF Bistability Phenomenon
N. Guihery, J.-P. Malrieu, D. Maynau, and K. Hendrick 45

Traces of Spin-Adapted Reduced Density Matrices
E. Pérez-Romero, L. M. Tel, and C. Valdemoro 55

Average Energy of an *N*-Electron System in a Finite-Dimensional and Spin-Adapted Model Space
J. Karwowski, J. Planelles, and F. Rajadell 63

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Nonempirical Wave Functions for Very Large Molecules. II. The PRDDO/M/FCP Method
A. Derecskei-Kovacs, D. E. Woon, and D. S. Marynick 67

Maximum-Entropy Analysis of Momentum Densities in Diatomic Molecules
J. Antolín, A. Zarzo, J. C. Angulo, and J. Cuchí **77**

The Relative Performance of the Local Density Approximation and Gradient-Corrected Density Functional Theory for Computing Metal–Ligand Distances in Werner-Type Organometallic Complexes
M. R. Bray, R. J. Deeth, V. J. Paget, and P. D. Sheen **85**

Electron Affinities of Metals Computed by Density Functional Theory and Ab Initio Methods
B. S. Jursic **93**

CFPHGLF Calculation of ^3S Excited States for Heliumlike Three-Body Systems
Y. Wang and C. Deng **101**

Accurate Nonrelativistic Energies for $^2P^o$ *States of the Li* Isoelectronic Series
R. Barrois, H. Kleindienst, and A. Lüchow **107**

Nonempirical Ab Initio Studies on Inner-Sphere Reorganization Energies of $M^{2+}(H_2O)_6/M^{3+}(H_2O)_6$ Redox Couples at Valence Basis Level
Y. Bu, Y. Ding, F. He, L. Jiang, and X. Song **117**

Molecular Structure, Dynamics, and Function of Biological Systems

Theoretical Study of the Stereoisomers of Tetrahydrocannabinols
N. S. Bodor and M.-J. Huang **127**

Ab Initio MO Study of the Chlorophyll Dimer in the Photosynthetic Reaction Center. I. A Theoretical Treatment of the Electrostatic Field Created by the Surrounding Proteins
T. Sakuma, H. Kashiwagi, T. Takada, and H. Nakamura **137**

Erratum

Valence Energy in Variational Monte Carlo: CuH Dissociation Energy
S. M. Rothstein **153**

Announcement **155**

Diskette Submission Instructions ..... **I**

Issue No. 2, 1997

Special Issue: VIth International Conference on the Applications of Density Functional Theory
Guest Editors:
Henry Chermette, Annick Goursot, and Claude Mijoule
(Part I of III)

Theoretical and Computational Developments

Introduction
A. Goursot **157**

List of Participants **159**

Charge Response Criteria of Chemical Reactivity: Fukui Function Indices and Populational Reference Frames Reflecting the Interreactant Charge Coupling
R. F. Nalewajski **181**

On-Top Pair-Density Interpretation of Spin Density Functional Theory, with Applications to Magnetism
J. P. Perdew, M. Ernzerhof, K. Burke, and A. Savin **197**

Incorporating Solvation Effects into Density Functional Theory: Calculation of Absolute Acidities
W. H. Richardson, C. Peng, D. Bashford, L. Noodleman, and D. A. Case **207**

Symmetrical "Nonproduct" Quadrature Rules for a *Fast* Calculation of Multicenter Integrals
C. Daul and S. Daul **219**

Direct Approximation of the Long- and Short-Range Components of the Exchange–Correlation Kohn–Sham Potential
O. V. Gritsenko, R. Van Leeuwen, and E. J. Baerends **231**

Differences Between Ab Initio and Density Functional Electron Densities
E. Ortiz-Henarejos and E. San-Fabían **245**

Density Functional Study of Atomic Electron Affinities Using a Nonlocal Exchange and a Local Correlation Functional
N. A. Cordero and J. A. Alonso **253**

Exact Exchange–Correlation Potential from Low-Order Density Matrices
A. Holas and N. H. March **263**

Simplified Accurate Approximation for the Kohn–Sham Potential Using the KLI Method
J. B. Krieger, Y. Li, Y. Liu, and G. J. Iafrate **273**

Additive Density Functional Correlation Corrections to Single Particle Theories
M. Levy **281**

Why the Generalized Gradient Approximation Works and How to Go Beyond It
K. Burke, J. P. Perdew, and M. Ernzerhof **287**

DFT–LDA Pseudopotentials in Quantum Monte Carlo
M. Menchi and A. Bosin **295**

Kohn–Sham Equations with Constrained Electron Density: The Effect of Various Kinetic Energy Functional Parametrizations on the Ground-State Molecular Properties
T. A. Wesolowski and J. Weber **303**

New Functionals for Correlation Energy Deduced in the Framework of the Correlation Factor Approach
F. Moscardó and A. Pérez-Jiménez **313**

Density Functional Theory for Triplet Superconductors
K. Capelle and E. K. U. Gross **325**

Density Functional Theory for Excited States and Special Symmetries
A. K. Theophilou **333**

Multigrid Methods in Density Functional Theory
T. L. Beck, K. A. Iyer, and M. P. Merrick **341**

Diagonalization Free Implementation of Kohn–Sham Equations with Localized Basis Sets
V. Termath **349**

Translational and Rotational Invariance Requisites for Density Functional Derivatives
D. P. Joubert **355**

Diskette Submission Instructions ..... **I**

Issue No. 3, 1997

Special Issue: VIth International Conference on the Applications of Density Functional Theory

Guest Editors:

Henry Chermette, Annick Goursot, and Claude Mijoule

(Part II of III)

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Comparison Between Post-Hartree–Fock and DFT Methods for the Study of Strength and Mechanism of Cleavage of Hg—C Bond
V. Barone, A. Bencini, F. Totti, and M. G. Uytterhoeven **361**

Ab Initio Molecular Dynamics Calculations to Study Catalysis
K. Schwarz, E. Nusterer, P. Margl, and P. E. Blöchl **369**

Density Functional Study of Diels–Alder Reactions Between Cyclopentadiene and Substituted Derivatives of Ethylene
V. Branchadell **381**

Density Functional Analysis of a Decomposition of 4-Nitro-1,2,3-Triazole Through the Evolution of N_2
P. Politzer, M. E. Grice, and J. M. Seminario **389**

Acid–Base Catalysis in Zeolites from First Principles
R. Shah, M. C. Payne, and J. D. Gale **393**

Assignment of Photoelectron Spectra by the Help of Density Functional Calculations
L. Nyulászi and T. Veszprémi **399**

Molybdenum(VI) Dioxodihalides: Agreement with Experiment and Prediction of Unknown Properties Through Density Functional Theory
M. Torrent, P. Gili, M. Duran, and M. Solà **405**

Density Functional Potential Energy Hypersurface of Protonated Ozone: A Comparison Between Different Gradient-Corrected Nonlocal Functionals
J. Rubio, N. Russo, and E. Sicilia **415**

Hardness Conservation as a New Transferability Criterion: Application to Fully Nonlocal Pseudopotentials
A. Filippetti, A. Satta, D. Vanderbilt, and W. Zhong **421**

Toward a General Protocol for the Study of Static and Dynamic Properties of Hydrogen-Bonded Systems
V. Barone and C. Adamo **429**

First-Row Transition-Metal Hydrides: A Challenging Playground for New Theoretical Approaches
V. Barone and C. Adamo **443**

Density Functional Theory Study on Molecular Structure and Vibrational IR Spectra of Isocytosine
J. S. Kwiatkowski and J. Leszczynski **453**

A Density Functional Study of Fe—N_2, Fe—N_2^+, and Fe—N_2^-
A. Zacarías, H. Torrens, and M. Castro **467**

A Density Functional Study of Ground-State and Excited-State Properties of $CoAl_2Cl_8(g)$
K. G. Doclo, C. A. Daul, and S. Creve **475**

Thermochemical Data Relative to the Complex Formation in Gas Phase Derived from Computational Chemistry
A. Hemery, G. Picard, M. Sibony, and B. Champin **483**

Application of Second-Order Density Functional Methods to the Calculation of the BeFH Potential Energy Surface
A. Aguado, V. Sanz, and M. Paniagua **491**

Acidic and Basic Molecular Hardness in LCAO Approximation
R. Balawender, L. Komorowski, and S. Roszak **499**

Computational and Analytical Chemistry: Methodology to Study Chemical Reactions Between Sodium, Calcium, and Aluminum Fluorides in Molten Cryolite
F. Bouyer, G. Picard, and J.-J. Legendre **507**

Systematic Study of the Lowest Energy States of Pd, Pd_2, and Pd_3
J. M. Seminario, A. G. Zacarías, and M. Castro **515**

Analytical Schwartz Density Applied to Heavy Two-Electron Ions
E. Romera, J. S. Dehesa, and T. Koga **525**

Density Functional Calculations on Jahn–Teller Effect of Tetrachloromethane Cation
J. M. Garcia De La Vega, B. Miguel, and E. San Fabian **533**

Modeling of the Hydration Sphere of Gadolinium(III) Ion Using Density Functional Theory
O. Schafer and C. Daul **541**

Are Metal–CO Molecules Linear? ScCO, TiCO, VCO, and CrCO Cases Studied in MRCI Method Compared with DFT Method
G.-H. Jeung and S. Haettel **547**

Numerical Evaluation of the Internal Orbitally Resolved Chemical Hardness Tensor in Density Functional Theory
M. Grigorov, J. Weber, H. Chermette, and J. M. J. Tronchet **551**

A Microscopic Insight into Oscillator Strengths: The Charge Transfer Bands for $CuCl_4^{2-}$
M. Barriuso, J. Aramburu, C. Daul, and M. Moreno **563**

Density Functional Investigation of the Molecular Geometries, Harmonic Vibrational Frequencies, Singlet–Triplet Energy Separations, Adiabatic Ionization Potentials, and Electron Affinities of XY_2(X = Si, Ge, Sn; Y = F, Cl) Systems
E. Sicilia, M. Toscano, T. Mineva, and N. Russo **571**

Density Functional Calculations of Optical Excitation Energies by a Transition-State Method
A. Stückl, C. A. Daul, and H. U. Güdel **579**

Two-Electron Valence Indices from the Kohn–Sham Orbitals
R. F. Nalewajski, J. Mrozek, and A. Michalak **589**

Diskette Submission Instructions ..... **I**

Issue No. 4, 1997

Special Issue: VIth International Conference on the Applications of Density Functional Theory
Guest Editors:
Henry Chermette, Annick Goursot, and Claude Mijoule
(Part III of III)

Properties, Dynamics, and Electronic Structure of Condensed Systems and Clusters

Density Functional Theory and Pseudopotentials: A Panacea for Calculating Properties of Materials
M. L. Cohen **603**

Ionic Vibrational Breathing Mode of Metallic Clusters
J. G. Aguilar, A. Mañanes, F. Duque, M. J. López, M. P. Iñguez, and J. A. Alonso **613**

Neutral Atoms in Ionic Lattices: Study of KCl:Ag^0
I. Cabria, M. T. Barriuso, J. A. Aramburu, and M. Moreno **627**

LDA Electronic Structure Calculations on Au_{13} Cluster
L. Lamare and F. Michel-Calendini **635**

Benchmark Comparison of Gradient-Dependent and Local Density Calculations for Bulk Silicon and Aluminum
S. B. Trickey **641**

All-Electron Calculations with Plane Waves in Solid Lithium Hydride
L. Bellaiche and K. Kunc **647**

Impurity Levels and Nonlinear Optical Properties of Doped $BaTiO_3$ from Extended Cluster LDA Calculations
M. Actis and F. Michel-Calendini **657**

Solvent Effects Computed with the Gaussian Density Functional Method
T. Mineva and N. Russo **665**

Density Functional Study on the Activation of Methane Over Pd_2, PdO, and Pd_2O Clusters
E. Broclawik, R. Yamauchi, A. Endou, M. Kubo, and A. Miyamoto **673**

Density Functional Investigation of the Mechanism of the Selective Catalytic Reduction of NO by NH_3 Over Vanadium Oxide Model Clusters
F. Gilardoni, J. Weber, and A. Baiker **683**

Comparative Study of DFT(LSD-CGA) and RHF Molecular Structures of Quinoid and Aromatic Model Systems for Head-to-Tail Electroactive Polymers
A. Grand, F. Jolibois, J. P. Denis, and J. Delhalle **689**

Nonlinear Response of Aluminum Surface to Electric Field
A. Kiejna **699**

Local Density Functional Calculations of the Electronic Structures of the Intermetallic Systems U_2Fe_2Sn and UFe_2Ge_2
S. F. Matar, V. Eyert, B. Chevalier, and J. Etourneau **705**

Simulation of Tungsten Tip-Al(100) Surface Electronic Structure Through LCAO–LSD Calculations
L. Lamare and F. Michel-Calendini **711**

Ab Initio Study of Epitaxial Growth on Stepped Si(100) Surface
V. Milman **719**

Molecular Structure, Dynamics, and Function of Biological Systems

Density-Functional Methods for the Study of the Ground-State Vibrations of the Guanidinium Ion
A. L. Magalhães and J. A. N. F. Gomes **725**

Guidelines for Electronic Submission ..... **I**

Issue No. 5, 1997

Theoretical and Computational Developments

Overlapping Shells Model Applied to Diamondlike Crystals
A. Kolezynski, W. S. Ptak, and K. Tkacz-Smiech **741**

Symmetric Group Approach to Relativistic CI. IV. Representations of One-Electron Spin Operators and Their Products in a Symmetric Group-Adapted Basis of *N*-Electron Spin Functions
N. Flocke **747**

A Fourier–Bessel Expansion for Solving Radial Schrödinger Equation in Two Dimensions
H. Taseli and A. Zafer **759**

Completeness Criteria for Explicitly Correlated Gaussian Geminal Bases of Axial Symmetry
B. Jeziorski, R. Bukowski, and K. Szalewicz **769**

A New Iterative Method for Solving the Time-Independent Schrödinger Equation Based on the Generalized Bloch Equation. I. Boson Systems: The Quartic Anharmonic Oscillator
H. Meißner and E. O. Steinborn **777**

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Peptide Models. XIV. Ab Initio Study on the Role of Side-Chain Backbone Interaction Stabilizing the Building Unit of Right- and Left-Handed Helices in Peptides and Proteins
A. Perczel, Ö. Farkas, J. F. Marcoccia, and I. G. Csizmadia **797**

Theoretical Studies on the Structures and Electronic Spectra of $C_{70}CH_2$
Q. Teng, X. Zhao, Z.-S. Cai, and A. C. Tang **815**

Cloppa RPA–AM1 Analysis of the Anisotropy of NMR $^1J(XY)$ Coupling Tensors in Me_3XY Compounds ($X = {}^{13}C, {}^{29}Si, {}^{119}Sn, {}^{207}Pb$; $Y = {}^{19}F, {}^{35}Cl$)
J. A. González, G. A. Aucar, M. C. Ruiz de Azúa, and R. J. Contreras **823**

Density-Gradient Analysis for Density Functional Theory: Application to Atoms
A. Zupan, J. P. Perdew, K. Burke, and M. Causà **835**

Conductivity in Polyacetylene. IV. Ab Initio Calculations for a Two-Site Model for Electron Transfer Between Allyl Anion and Allyl
L. Rodriguez-Monge and S. Larsson **847**

The Effect of an Electric Field on the Vibrational Frequency of CN
C. W. Bauschlicher, Jr. **859**

Molecular Structure, Dynamics, and Function of Biological Systems

Theoretical Investigation of the Rates of Electron Transfer Processes $Q_I^- + Q_{II} \rightarrow Q_I + Q_{II}^-$ and $Q_I^- + Q_{II}^- \rightarrow Q_I + Q_{II}^{2-}$ in Photosynthesis
S. N. Datta and B. Mallik **865**

Guidelines for Electronic Submission ..... **I**

Issue No. 6, 1997

Theoretical and Computational Developments

Comprehensive Strategy for the Calculation of Overlap Integrals with Slater-Type Orbitals
H. W. Jones **881**

Design of an Exchange Functional with Correct Asymptotics
R. Santamaria **891**

Calculation of NMR Shielding Tensors Based on Density Functional Theory and a Scalar Relativistic Pauli-Type Hamiltonian. The Application to Transition Metal Complexes
G. Schreckenbach and T. Ziegler **899**

Substitution Effects by SCF and Hückel Theory
M. Grayson **919**

Addendum to Construction of Linearly Independent Relativistic Symmetry Orbitals for Finite Double-Point Groups Including Time-Reversal Symmetry
J. Meyer **929**

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Correlation Entropy of the H_2 Molecule
P. Gersdorf, W. John, J. P. Perdew, and P. Ziesche **935**

Optimized Gaussian Basis Sets for Use with Relativistic Effective (Core) Potentials: K, Ca, Ga—Kr
J.-P. Blaudeau and L. A. Curtiss **943**

An Ab Initio Study of the Structure, Dissociation Energy, and Heat of Formation of Na_2S
Y. Zhao, T. Gu, S. Pan, and J. Sun **953**

Theoretical Studies on Local Anesthetics: Procaine, Lidocaine, Tetracaine, Bupivacaine, and Dibucaine—Neutral and Monoprotonated
J. Delphino Da Motta Neto and R. Bicca De Alencastro **959**

Structure and Energy of the Positively Ionized Water Clusters
Y. V. Novakovskaya and N. F. Stepanov **981**

Calculations of the Structure and Electronic Properties of Extended Polar Hydrocarbons
J. O. Morley **991**

Molecular Structure, Dynamics, and Function of Biological Systems

Electrostatic Medium Effects and Formal Quantum Structure–Activity Relationships in Apomorphines Interacting with D_1 and D_2 Dopamine Receptors
J. S. Gómez-Jeria and M. Ojeda-Vergara **997**

Volume Title Page **1003**

Author Index **1005**

Subject Index **1011**

Volume Table of Contents ..... **I**

Guidelines for Electronic Submission ..... **XIII**